

1,4-Dideoxy-1,4-iminothreitol  
90481-32-6 | DTXSID50238179

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.55

Global applicability domain: Inside

Local applicability domain index: 5.37e-01

Confidence level: 8.35e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N-(Hydroxyethyl)ethylenediamine</div> <div>Measured: 2.88</div> <div>Predicted: 3.29</div>	<div>Image not found</div> <div>1,1'-Oxybis-2-propanol</div> <div>Measured: 4.57</div> <div>Predicted: 3.83</div>	<div>Image not found</div> <div>Diethylenetriamine</div> <div>Measured: 4.47</div> <div>Predicted: 4.05</div>
<div>Image not found</div> <div>Cyanoguanidine</div> <div>Measured: 3.09</div> <div>Predicted: 2.93</div>	<div>Image not found</div> <div>Amitrole</div> <div>Measured: 3.09</div> <div>Predicted: 3.40</div>	